7.0 MODELING 2016 ADDENDUM

As noted in the 2016 Geology (Section 4.0) addendum, the WDW-164 and WDW-165 Injection Intervals are being combined for this Petition reissuance into one composite Injection Interval is to address the upward (outside of the casing) movement of wastewater in WDW-164 as noted from recent years' Mechanical Integrity testing. By combining the two previously separate Injection Intervals into one composite WDW-164/WDW-165 Injection Interval, this upward movement now remains within the newly defined composite WDW-164/WDW-165 Injection Interval. To compensate for the inability to adequately quantify the amount of fluid movement entering the overlying (currently defined) WDW-165 Injection Interval, the composite Injection Interval's maximum injection rate will be reduced to 500 gpm from the 1,000 gpm into the two previously separate Injection Intervals. This allows the current (2009 submission) lateral and vertical model (plume and pressure) demonstrations for the composite Injection Interval to remain valid and very conservative.

The proposed Injection Zone depths remain the same for the composite Injection Interval (4,715 to 8,250 feet KB) and for the WDW-163 Injection Interval (4,725 to approximately 8,250 ft KB). The composite WDW-164/WDW-165 Injection Interval is now defined as from a base at 8,005 feet KB (open hole log from WDW-164 1-17-81 Schlumberger Dual Induction-SFL Compensated Neutron – Formation Density Log) to a top at 6,600 feet KB (open hole log from WDW-165 3-8-81 Induction-SFL Compensated Neutron – Formation Density Log) and to a top at 6,595 feet KB (open hole log from WDW-164 1-17-81 Schlumberger Dual Induction-SFL Compensated Neutron – Formation Density Log). The updated Figure 4-7 illustrates the proposed composite WDW-164/WDW-165 Injection Interval defined depths, as well as those of the WDW-163 Injection Interval.

Although the WDW-164 and WDW-165 Injection Intervals are being combined, the modeled net sand thickness values for each injection Interval have not been combined

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into a single modeled net thickness isopach, but remain split to retain the two original models' variable thickness and variable structure values. Current WDW-164 and WDW-165 Injection Interval lateral plume model thickness values reflect these isopach map thicknesses, and as these models continue to demonstrate conservative plume movements within each interval, the isopach maps have not been changed. Variable thicknesses are used in both the SWIFT pressure and transport models across the areas of the model grids, representative of the mapped thicknesses as presented in each of the geologic isopach maps.

The projected maximum injection rates of 500 gpm into each of the current WDW-164 and WDW-165 Injection Intervals have been retained for both intervals' models, as this conservatively overestimates the future injection volume into the proposed composite WDW-164/WDW-165 Injection Interval. As noted earlier, the proposed composite Injection Interval will have a maximum 500 gpm injection rate, which is one half of the combined maximum injection rate of the individual WDW-164 and WDW-165 Injection Intervals. These current (2009) models increased future injection rates to 500 gpm into each interval, beginning on 1/1/2008, with projected maximum injection rates continuing to the end of the modeled operational period (12/31/2017).

The maximum permeability for the WDW-163 lateral plume models is currently 1,600 mD, and the minimum permeability used in these models is 500 mD. The maximum permeability for the WDW-164 lateral plume models is 400 mD, and the minimum permeability used in these models is 40 mD. The maximum permeability for the WDW-165 lateral plume models is 147 mD, and the minimum permeability used in these models is 33 mD (all three ranges are the same as in the previous Petition demonstration). On the high end, these selections maximize the low- and high-density plume movements. The low end values are used in the SWIFT pressure models to ensure the maximum calculated pressure increases.

An updated Table 7-3 is attached, which incorporates the results of fall-off testing performed on the three Ineos injection wells since the 2008 Petition reissuance submittal.

For WDW-163, the derived permeability values for 2009 (2,348 mD) and 2011 (41 mD) are outside of the modeled range (500 to 1,600 mD), but are considered outliers and not representative of the historical Injection Interval permeability. For WDW-164, all of the post-2008 derived permeability values are within the modeled range (40 to 400 mD). For WDW-165, all of the post-2008 derived permeability values are within the modeled range (33 to 147 mD). Relevant summary tables and figures from the 2009 through 2015 fall-off test reports are attached for inclusion into Appendix G.

Updated flowing and static bottom-hole pressure data for the three Injection Intervals since the 2008 Petition submittal was gathered from historical fall-off test analyses. This information is provided in the attached Table 7-5a. The flowing pressures (as shown on Table 7-5a) were converted to the three Injection Intervals' SWIFT pressure model reference depths (depths to center of grid block at each Ineos well location). These values indicate that the SWIFT pressure models remain conservative for this updated historical period, and are also conservative for future pressure increase calculations due to the models' incorporation of maximum permitted well injection rates through the projected operational periods. The projected SWIFT model pressure increases in the three Injection Intervals is shown in Table 3-1 and Figure 3-4 of the 2009 Petition submittal. This table and figure show the modeled flowing bottom-hole pressures at the reference depths for the WDW-163, WDW-164, and WDW-165 to be approximately 2,460 psi, 4,010 psi, and 3,610 psi respectively over the 2009-2015 time period.

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7.0 MODELING

Information regarding the geologic, hydrogeologic, and geochemical data of site conditions, and the waste stream characteristics at Ineos was presented in earlier sections. That information is used in this section to provide a demonstration, via model simulation, that injected wastes will not migrate to a point outside the permitted Injection Zone within a period of 10,000 years. A discussion of the modeling approach and methodology is presented below.

7.1 Model Objectives and Approach

The modeling performed herein specifically addresses two considerations in order to demonstrate no-migration:

1. Injection Interval pressurization during the operational period; and
2. Lateral and vertical waste transport and containment within the Injection Zone during the 10,000-year post-operational period.

To meet these objectives, four separate models were constructed using different approaches. Each model addresses specific considerations for a demonstration of no-migration. The descriptions and approaches of the four models are shown in Table 7-1.

The Sandia Waste Isolation Flow and Transport (SWIFT) code was employed in the lateral (numerical) models. The lateral models are two-dimensional, variable density, and incorporate the geologic structure (elevation) and thickness of the Injection Interval, as defined in Section 4.0. There is, however, no vertical transport allowed outside of the model Injection Interval, thereby maximizing the Injection Interval pressurization and lateral waste transport.

Analytical techniques were used in the vertical transport model. In accordance with 40 CFR §148.21(a)(3) and (5), the numerical and analytical models used to demonstrate no migration have been verified and validated. The models are available to the public and are based on sound engineering and hydrogeologic principles.

7.1.1 The SWIFT Computer Code

The computer simulation code used for modeling the pressure buildup and lateral migration of injected waste at Ineos is SWIFT for Windows (HSI Geotrans, 2000). SWIFT for Windows is a version of the SWIFT code (Reeves and others, 1986; Finley and Reeves, 1982; Ward and others, 1987; Reeves and Ward, 1986; Intercomp, 1976). SWIFT was originally called SWIP (Survey Waste Injection Program) and was developed under contract to the U.S. Geological Survey (Intercomp, 1976). The code was developed to model waste injection in deep brine aquifers under conditions of variable fluid density, viscosity, and temperature.

SWIFT is a three-dimensional finite difference code that can be used to simulate ground water flow, contaminant transport, and heat transport in single or dual porosity media. Steady state or transient conditions can be simulated. In SWIFT, the equations governing groundwater flow and solute transport are coupled through: 1) the pore fluid velocity; 2) the dependence of the fluid density on pressure, solute mass fraction and temperature; and 3) the dependence of fluid viscosity on solute mass fraction and temperature.

SWIFT has been extensively verified and validated. Ward and others (1984) documented the benchmarking of SWIFT against eleven analytical solutions and field problems. These problems explore a wide range of SWIFT's capabilities including variable density flow and disposal well injection. Illustrative problems using the SWIFT code have been published in two reports (Finley and Reeves, 1982; Reeves and others, 1987).

7.1.2 Analytical Model

The vertical transport of waste and dissolved waste constituents was calculated using an analytical model. This model incorporated the effects due to both advection and molecular diffusion. The advective transport arises from the Injection Interval pressure buildup during the operational period, and the buoyant gradient resulting from the density contrast between the injectate and formation fluid. The molecular diffusion component of transport results from the concentration gradient between the Injection Interval and the overlying strata. Additionally, the diffusive transport through a mud-filled borehole is calculated to address the possibility of a mud-filled artificial penetration intersecting the Injection Interval and plume.

The analytical solutions are derived from published materials and employ sound hydrogeologic principles. Derivations and discussions of the mathematical models used in the vertical transport of waste are presented in Section 7.5.

7.2 General Modeling Methodology and Assumptions

In this modeling, a "conservative approach" methodology was applied. Model input parameters, initial conditions, and boundary conditions were employed to ensure that the simulated Injection Interval pressurization and waste transport distance are over-estimated. The general methods employed to ensure conservative modeling results are discussed below. Information regarding the specifics of each model is presented in the appropriate model discussions.

Ineos uses its injection wells to inject into the upper and middle Frio Formation sands through perforated long string casings or screens across the three permitted Injection Intervals: 5,370 – 5,710 feet KB (WDW-163), 6,600 – 7,500 feet KB (WDW-165), and 7,435 – 8,005 feet KB (WDW-164). Separate models for each of the three Injection Intervals have been constructed and are presented in this section.

The Injection Interval grid block centers are located in the lateral models at depths of 5,501 feet (at WDW-163), 7,766 feet (at WDW-164), and 7,214 feet (at WDW-165). The tops of the Injection Intervals for the vertical models are placed at the current Injection Interval tops of 5,370 feet (WDW-163), 7,435 feet (WDW-164), and 6,600 feet (WDW-165). These vertical model top values are conservative, since the actual perforated/screened interval tops in these wells are substantially below the modeled Injection Interval tops.

For purposes of this demonstration, all modeled flows into the Ineos wells inject into each Injection Interval sand at 500 gpm (per well) for a projected period of ten years, in order to maximize the pressure increases at the modeled wells. The future injection rates are set at the maximum permitted rates for each injection well.

Regional structural information was incorporated into the lateral transport models to address the possibility of "updip" or "downdip" movement of injected wastes that have a density different than the native formation fluid. The transport models include the effects of advection, dispersion, and molecular diffusion. The maximum injectate density was used in each Injection Interval pressurization model and each high-density injectate transport model to maximize pressure buildup and downdip waste transport. The minimum injectate density was used in the low-density injectate lateral transport models and the vertical transport models to maximize updip and vertical movement. Formation structural information was not incorporated into the vertical transport model, thereby maximizing the upward driving forces of pressure buildup and buoyancy at the point of maximum concentration (wellbore).

No effects from other injection wells have been incorporated into the models. There is one Class II salt water disposal well (Map ID No. 70, formerly an oil well now injecting into the same perforations) located within the Ineos composite 2-mile radius AOR. This well currently has perforations between 5,428 feet and 5,433 feet, and injects salt water into a thin sand between Sands 3 and 4 of the WDW-163 Injection Interval. Also, no effects from oil or gas production wells have been incorporated into the models, as there are no known producing horizons correlative with the Ineos Injection Intervals within the AOR or areas of the modeled plumes.

7.2.1 Geologic and Hydrologic Model Assumptions

Several hydrologic and geologic assumptions were made in the modeling portion of this petition. General assumptions required for both the lateral SWIFT and vertical models are: 1) Darcy's law is valid, i.e. ground water flow is laminar; 2) the porous medium is fully saturated and confined; 3) hydrodynamic dispersion can be described as a Fickian process; 4) the initial model concentration is zero; 5) the injected and formation fluids are miscible and no reactions between waste constituents or between waste and formation or formation fluids occur; and 6) the waste movement is modeled by considering the movement of a single conservative species, i.e., no sorption or decay of the waste occurs. Specific assumptions pertaining to each model are detailed in the following sections.

7.2.2 Modeled Concentration Reduction

A 4.0 x 10^9-order of magnitude (4,000,000,000-fold) reduction in the initial concentration was used to define the limits of migration of hazardous constituents. This reduction is based on a maximum concentration measurement of constituents present in the waste stream. An additional increase above the maximum historically measured concentration was applied to provide a conservative result. At this level of reduction, hazardous waste constituents in the Ineos waste stream will have been conservatively reduced to levels which are below the accepted health based limits for those constituents. Table 6-1 presents a summary of the hazardous waste constituents (maximum anticipated concentration) in the Ineos waste stream, USEPA health based limits for the subject compounds, and the magnitude of reduction necessary to lower maximum anticipated concentrations below existing health based limits. The constituent acrylamide, the worst-case constituent on which the currently approved Petition was modeled, will continue to be the worst case hazardous constituent for modeling purposes.

7.2.3 Boundary Conditions

The geologic area of review indicates that the Frio Injection Intervals are variable in thickness surrounding the facility. In the lateral transport and Injection Interval pressurization models, all lateral boundaries are "open" to maximize waste movement. This is accomplished by imposing Carter-Tracy boundaries on all sides of the model. The exception to this is the WDW-163 Injection Interval model, where the sand pinchout updip has been modeled by using a no-flow boundary at the north edge of the expanded model.

The "top" and "bottom" of the Injection Intervals in the lateral models are non-transmissive, with the assignment of zero hydraulic conductivity in the z-direction. This confines waste movement and Injection Interval pressurization to the modeled Injection Interval thickness. This is a conservative condition because no waste transmission or pressure leakage beyond the Injection Interval can occur. This approach maximizes lateral waste movement and pressure buildup within the Injection Interval.

In the vertical model, all transport is directed upward from the modeled tops of the three Frio Injection Intervals. The transport models are 1-dimensional with no transverse component of velocity or dispersivity. Again, this approach maximizes vertical waste movement.

7.3 Model Input Parameters

The input values used in the lateral and vertical models are presented in Tables 7-2a (WDW-163), 7-2b (WDW-164), and 7-2c (WDW-165). The parameters employed in these models are based on data representative of actual reservoir conditions. If no data were available, the input values were selected conservatively to result in maximum Injection Interval pressurization and waste transport distances. Additional discussion is given below for each model input parameter.

7.3.1 Injection Interval Depth, Structure and Thickness

Depth

The Injection Interval tops at the modeled Ineos wells have been set at (for the lateral models) or above (for the vertical models) the effective tops of the three Frio Injection Interval sands (5,422 feet KB at WDW-163, 7,435 feet KB at WDW-164, and 6,750 feet KB at WDW-165), which is conservative, because the perforated/screened interval in

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each well may be deeper but is not shallower than those points. The perforated/screened intervals are all at or below the correlated tops of the three Frio Injection Intervals.

Structure

Each lateral SWIFT model incorporates variable structure (as opposed to a constant formation dip), where each node within the model domain is assigned a depth. The structural information used in the modeling is based on the regional geologic study area at Ineos, as discussed in Section 4.0. The geologic data used to generate the Injection Interval structure maps was incorporated into the SWIFT input files. The resulting Frio structures in SWIFT are shown on Figures 7-1, 7-2, and 7-3. The contoured geologic structure maps on the tops of the upper and middle Frio Formation are presented on Plates 4-7 and 4-9. In comparing the geologic and model contours maps, it is evident that the structural features are similar although they may be offset vertically by up to several hundred feet. Structural trends are similar between the geologic and model maps within the areas of the plumes. Therefore, the Frio structures have been correctly incorporated into the SWIFT models.

Thickness

In each lateral model, the Injection Interval thickness is assigned to be the net Frio interval thickness as measured from subsurface well control in the mapped area. This information was incorporated into the SWIFT model in the same fashion as described above for the depth information. The geologic data used to generate the thickness maps was incorporated into the SWIFT input files. The resulting net thicknesses in SWIFT are shown in Figures 7-4, 7-5, and 7-6, in comparison to the original contoured isopach maps provided as Plates 4-8, 4-10, and 4-11. From inspection of the contours maps, it can be concluded that there is no significant difference within the overlaid contoured areas within the areas of the AOR and light plumes. Therefore, the Frio thickness information has been correctly incorporated into the models.

Based on the geologic mapping presented in Section 4.0, the three Frio Injection Intervals have minimum net sand thickness values at the Ineos wells of 98 feet (WDW-163), 338 feet (WDW-164), and 550 feet (WDW-165), respectively. WDW-163 is completed through perforated casing across the 86 net feet of Sand 3 and 174 feet of Sand 4 of the WDW-163 Injection Interval, totaling 260 net feet of sand. The thickness at WDW-163 was assigned to be 98 feet for that Injection Interval, ignoring the majority of the perforated thickness in Sand 4. Across the mapped area, the Sand 3/Sand 4 net sand thickness values (0 to 660 feet) reflect the interval over which the injectate could be emplaced by the petitioned well in the Sand 3/Sand 4 lateral transport model. WDW-164 is completed using a screen and gravel pack into the WDW-164 sand, with 483 feet of screen present across 360 net feet of sand. The thickness at WDW-164 was assigned to be 338 feet for that Injection Interval. The correlated thickness values of the WDW-164 sand (150 to 600 feet) across the mapped area reflect the interval over which the injectate could be emplaced by the petitioned well in the WDW-164 lateral transport model. WDW-165 is completed using a screen and gravel pack into the WDW-165 sand, with 687 feet of screen present across 550 net feet of sand. The thickness at WDW-165 was assigned to be 550 feet for that Injection Interval. Across the mapped area, the WDW-165 net sand thickness values (290 to 620 feet) reflect the interval over which the injectate could be emplaced by the petitioned well in the WDW-165 lateral transport model.

Plates 4-8, 4-10, and 4-11 are net thickness maps of the WDW-163, WDW-165, and WDW-164 effective Injection Intervals, respectively. The isopach maps were constructed based on net sand thickness values for each Injection Interval acquired from open hole electric logs of wells within the mapped area. The modeled sand thickness value used at WDW-163 of 98 feet is less than the actual net Injection Interval sand thickness of both Sands 3 and 4 at that well, reflecting that Sand 3 is taking the majority of the well flow. Once Sands 3 and 4 merge in downdip (as shown on the dip cross-section Plate 4-1), the net thickness of both sands combined is included in the Plate 4-8 isopach map, but updip from that point only the thickness values of Sand 3 are incorporated into the isopach map.

This was done to provide a conservatively large light plume movement and pressure increase over the modeling period, since all injectate into WDW-163 was directed into Sand 3, which pinches out significantly farther updip than Sand 4. The WDW-163 effective Injection Interval isopach consists of Sand 3 only updip of its coalescing with Sand 4. The Plates 4-10 and 4-11 isopach maps of the WDW-165 and WDW-164 Injection Intervals are based on the net sand thicknesses found within those mapped horizons as delineated on the cross section Plates A-A′ and B-B′ (Plates 4-1 and 4-2). The Figure 4-7 cross section of the three Ineos injection wells highlights (by shading) the effective Injection Interval from which the net isopach maps were constructed.

Results from the available historic (1993-2008) radioactive tracer (RAT), temperature, and velocity shot log surveys at the Ineos wells indicate that the derived net receiving thickness values for each of the Injection Intervals is typically greater than that used in the Petition SWIFT modeling. Although only the velocity shot surveys are relatively accurate for determining net receiving interval thickness values, the RAT and temperature log surveys do provide indicators of minimum receiving thickness values. The RAT and temperature log surveys often tend to under-estimate the total receiving sand thickness due to a lack of sensitivity to zones receiving low flow.

For WDW-163, historic RAT surveys all indicate that the perforations remained uncovered by fill, and the reports note that at least 244 feet of net sand within that interval received flow during the annual testing. The only velocity shot survey (2001; included in Appendix J and discussed later in this section) indicated that 260 feet of sand was taking fluid, which is the thickness of the combined Sands 3 and 4 in the WDW-163 Injection Interval as seen on the open hole log. The three differential temperature log surveys also indicate minimum receiving thickness values of at least 244 feet.

For WDW-164, historic RAT surveys indicate that the perforations remained uncovered by fill except for the past three years, where flow also occurred into the fill. The reports note that at least 305 feet of net sand within that interval received flow during the annual testing. The only velocity shot survey (2001; included in Appendix J and discussed later in this section) indicated that 364 feet of sand was taking fluid, which is close to the 360 net feet of sand as estimated from the WDW-164 open hole log. The three differential temperature log surveys also indicate minimum receiving thickness values of at least 305 feet.

For WDW-165, historic RAT surveys indicate that the perforations remained uncovered by fill except for the past four years, where flow also occurred into the fill. The reports note that at least 467 feet of net sand within that interval received flow during the annual testing. The only velocity shot survey (2001; included in Appendix J and discussed later in this section) indicated that 492 feet of sand was taking fluid. The three differential temperature log surveys also indicate minimum receiving thickness values of at least 467 feet. The net receiving thickness values derived from the various available historic production log surveys reports have been summarized in Table 7-10. The relevant pages from the annual MIT reports discussing the production logging have also been added to Appendix J.

Velocity shot flow profile surveys were performed on the three Ineos injection wells during annual mechanical integrity testing performed in 2001. These surveys (included in Appendix J) give an indication of the wellbore flow profile and qualitatively indicate the overall fluid-receiving portion of each Injection Interval. The flow profile surveys indicate that WDW-163 is taking fluid through perforations over a net sand thickness of 260 feet, conservatively greater than the 98 feet assigned in the model. The flow profile surveys indicate that WDW-164 is taking fluid through the screened interval over a net sand thickness of 364 feet, conservatively greater than the 338 feet assigned in the model. The flow profile surveys indicate that WDW-165 is taking fluid through the screened interval over a net sand thickness of 492 feet, slightly less than the 550 feet assigned in the model. However, the interval not taking fluid (between 6,950 feet and 7,050 feet) includes an interval with two massive sands, which immediately above and below those depths are taking fluid. Thus the full thickness of these sands will continue to be counted as receiving fluid through vertical movement into these sands from the adjacent portions of these sands in the WDW-165 wellbore taking fluid. The sand thicknesses at the modeled wells for the three lateral models continue to conservatively reflect the minimum completion thicknesses.

7.3.2 SWIFT Hydraulic Conductivity and Permeability

A range of permeabilities and hydraulic conductivities was used in the lateral SWIFT models. The values were selected from available core and fall-off tests to encompass the range of permeability values present in the three Frio Injection Intervals. The results of the historical fall-off tests performed on the three Ineos injection wells are summarized in Table 7-3, and the data and reports included in Appendix G. Test data prior to 1994 (previous Petition re-issuance submittal) are limited to paper charts of those tests, copies of which are also included in Appendix G.

The maximum permeability for the WDW-163 lateral plume models was chosen to be 1,600 mD, and the minimum permeability used in these models was chosen to be 500 mD. The maximum permeability for the WDW-164 lateral plume models was chosen to be 400 mD, and the minimum permeability used in these models was chosen to be 40 mD. The maximum permeability for the WDW-165 lateral plume models was chosen to be 147 mD, and the minimum permeability used in these models was chosen to be 33 mD (both same as in previous Petition demonstration). On the high end, these selections maximize the low- and high-density plume movements. The low end values are used in the SWIFT pressure models to ensure the maximum calculated pressure increases. The values used in the SWIFT models are summarized in Tables 7-2a (WDW-163), 7-2b (WDW-164), and 7-2c (WDW-165). Hydraulic conductivity (as input into the SWIFT models) can be determined for a specified fluid and permeability by (Freeze and Cherry, 1979):

$$K = \frac{k \rho g}{\mu} \qquad \text{(Equation 7.1)}$$

where,	K	=	hydraulic conductivity, ft/day
	k	=	intrinsic permeability, ft^2
	ρ	=	fluid density, slugs/ft^3
	g	=	acceleration due to gravity, ft/sec^2
	μ	=	fluid viscosity, lb-sec/ft^2

A discussion of how the various hydraulic conductivities were determined is provided below.

7.3.2.1 Lateral Plume Model Permeability, Porosity, and Hydraulic Conductivity

WDW-163 Injection Interval

Full hole core samples were obtained during the drilling of WDW-163, and are included in Appendix E. The following core runs (CR) and samples were obtained:

Depth	Recovery	Stratigraphic Interval
CR1 4,900' – 4,918'	18' 3"	Anahuac Shale
CR2 5,340' – 5,360'	20'	upper Frio Sand No. 2
CR3 5,360' – 5,378'	18'	upper Frio Sand No. 2
CR4 5,600' – 5,618'	18'	upper Frio Sand No. 4

In addition to the full hole cores, 15 sidewall cores (included in Appendix E) were obtained between the depths of 4,720 feet and 5,725 feet. Analyses for permeability (to air) and porosity of 33 plugs removed from the full hole cores yielded a range in permeability between 770 mD and 7,200 mD for the sand intervals and a porosity range between 30 percent and 42.5 percent. The full hole core from CR1 (4,900 to 4,918 feet) was not tested because testing shale was not standard core laboratory practice at the time the well was installed.

Sidewall core analyses yield a porosity range from 20.4 percent in very fine grain shaley sand to 32.9 percent for silty sand. Air permeabilities ranged from 7.8 to 2,663 mD in the same core samples. Again, these values for sidewall core analyses are considerably lower than those for the full hole cores due to densification of the sidewall cores when collected.

The pressure modeling for the WDW-163 Injection Interval, 163pr34, employs a permeability value of 500 mD in order to provide a conservative (worst case) estimate of pressure buildup in the WDW-163 sands reservoir. This is equivalent to a hydraulic conductivity of 3.02 ft/day, based on a formation fluid density of 64.89 lb/ft^3, and a formation fluid viscosity of 0.47 cP at 158 °F. The low and high density lateral flow and transport models, 163lo32 and 163hi33, employ a permeability value of 1,600 mD in order to provide a conservative estimate of plume movement over 10,000/200 years, respectively. This is equivalent to a hydraulic conductivity of 9.68 ft/day, based on a formation fluid density of 64.89 lb/ft^3, and a formation fluid viscosity of 0.47 cP at 158 °F (see Section 7.3.7).

WDW-164 and WDW-165 Injection Intervals

Full-hole cores were obtained from WDW-164 (included in Appendix I) as follows:

Depth	*Recovered*	Stratigraphic Interval
CR1 6,962 - 6,982'	20'	middle Frio
CR2 7,416 - 7,426'	No Recovery	middle Frio
CR3 7,539 - 7,559'	20'	lower Frio
CR4 7,559 - 7,579'	6'	lower Frio

In addition to the full hole cores, 45 sidewall cores (included in Appendix E) were obtained between the depths of 6,620 feet and 8,038 feet. No full hole cores were obtained during the drilling of WDW-165. However, 45 sidewall cores were obtained between the depths of 5,300 feet and 7,435 feet. WDW-164 penetrated the effective Injection Intervals for both WDW-164 and WDW-165. Consequently, the core analyses results for these samples span both intervals. The ranges in values given below are based upon all core samples, whether taken from WDW-164 or WDW-165.

The air permeability and porosity based upon full hole core analyses samples from the WDW-164 effective Injection Interval, ranged, respectively, between 325 and 3,620 mD and 26.9 percent and 37.9 percent. Corresponding values for sidewall cores ranged between 3 and 428 mD and porosity between 20.1 percent and 32.3 percent, respectively. For reasons discussed previously, sidewall values are considerably lower.

Based upon full hole core sample analyses for the WDW-165 Injection Interval as taken from the WDW-164 well, the air permeability ranges between 442 mD and 2840 mD, and the porosity ranges between 29.7 percent and 36.4 percent. Sidewall core analyses yielded values of 31 mD (very shaley sand) to 1,495 mD for air permeability, and 21.6 to 32.5 percent for porosity. Again, the sidewall core analyses yield significantly lower values for permeability and porosity than the full hole core analyses.

The pressure modeling for the WDW-164 Injection Interval, 164pr42, employs a permeability value of 40 mD in order to provide a conservative (worst case) estimate of pressure buildup in the WDW-164 sands reservoir. This is equivalent to a hydraulic conductivity of 0.28 ft/day, based on a formation fluid density of 64.34 lb/ft^3, and a formation fluid viscosity of 0.40 cP at 192 °F. The low and high density lateral flow and transport models, 164lo40 and 164hi41, employ a permeability value of 400 mD in order to provide a worst case estimate of plume movement over 10,000/200 years, respectively. This is equivalent to a hydraulic conductivity of 2.82 ft/day, based on a formation fluid density of 64.34 lb/ft^3, and a formation fluid viscosity of 0.40 cP at 192 °F (see Section 7.3.7).

The pressure modeling for the WDW-165 Injection Interval, 165pr52, employs a permeability value of 33 mD in order to provide a conservative (worst case) estimate of pressure buildup in the WDW-165 sands reservoir. This is equivalent to a hydraulic conductivity of 0.22 ft/day, based on a formation fluid density of 64.51 lb/ft^3, and a formation fluid viscosity of 0.42 cP at 182 °F. The low and high density lateral flow and transport models, 165lo50 and 165hi51, employ a permeability value of 147 mD in order to provide a conservative estimate of plume movement over 10,000/200 years, respectively. This is equivalent to a hydraulic conductivity of 0.99 ft/day, based on a formation fluid density of 64.51 lb/ft^3, and a formation fluid viscosity of 0.42 cP at 182 °F (see Section 7.3.7).

7.3.2.2 Vertical Model Hydraulic Conductivity

The weighted average porosity and hydraulic conductivity are assumed homogeneous (no variation in permeability along the vertical path). Additionally, since the vertical model is one-dimensional (vertically upward), the weighted average porosity and hydraulic conductivity are assumed to be isotropic.

WDW-163 Injection Interval Vertical Hydraulic Conductivity

The containment interval hydraulic conductivity for the WDW-163 vertical model is based on average literature permeability values from Anahuac shales and measured sidewall/whole core values for the upper Frio sands. This containment interval contains 385 feet of Anahuac shale, underlain by 312 feet of inter-bedded Frio sand and shale strata, which overlays Sand 3 of the WDW-163 Injection Interval. The 697 feet thick containment interval consists of approximately 445 feet of shale, plus approximately 252 feet total thickness of sand. The shale strata are conservatively estimated to have permeabilities averaging 4.4×10^{-4} mD. This value is higher than the range provided for Gulf Coast shales by Clark (1988), and was determined from the harmonic average of four Gulf Coast shale core samples measured permeabilities (Conger, 1986). The sand strata are conservatively estimated to have a vertical permeability of 1,600 mD, equal to the maximum permeability used in the WDW-163 lateral model. In reality, vertical permeabilities in sands and shales typically are $1/10^{th}$ of the horizontal permeabilities.

In this model, the weighted average vertical permeability, k_z, of the containment interval is calculated using the method of Domenico and Schwartz (1990),

$$k_z = \Sigma\, b_i / \Sigma\, (b_i / k_i) \qquad \text{(Eq. 7.2)}$$

The weighted average permeability, k_z, is:

$$kz = \frac{445\,ft + 252\,ft}{\dfrac{445\,ft}{4.4 \times 10^{-4} mD} + \dfrac{252\,ft}{1{,}600\ mD}} = 6.9 \times 10^{-4} mD$$

This value was converted to a hydraulic conductivity of 4.12×10^{-6} feet per day with the following equation:

$$K = \frac{(0.00069 \text{ mD})(64.89 \text{ lb/ft}^3)(86{,}400 \text{ sec/day})(1 \text{ darcy})(1.06\times10^{-11} \text{ ft}^2\text{/darcy})}{(0.47 \text{ cP})(2.088\times10^{-5} \text{ lb-sec/ft}^2\text{-cP})(1{,}000 \text{ mD})}$$

$$K = 4.12 \times 10^{-6} \text{ feet/day}$$

The weighted average vertical hydraulic conductivity, Kz, is 4.12×10^{-6} feet/day using the formation fluid density of 64.89 lb/ft^3, and a formation fluid viscosity of 0.47 cP at 158 °F)

WDW-165 Injection Interval Vertical Hydraulic Conductivity

The containment interval for the WDW-165 Injection Interval vertical model is based on the same average permeability values from Anahuac and upper Frio sands and shales as described above. This containment interval is approximately 2,085 feet thick, and contains 385 feet of Anahuac shale, underlain by 1,700 feet of inter-bedded Frio sand and shale strata, which overlays the WDW-165 Injection Interval. The permeability values for the containment interval sands and shales are the same as described above. The 2,085 feet thick containment interval consists of approximately 975 feet of shale, plus approximately 1,110 feet total thickness of sand. The shale strata are conservatively estimated shale have permeabilities averaging 4.4×10^{-4} mD (discussed above), while the sand strata are conservatively estimated to have a vertical permeability of 1,600 mD, equal to the maximum permeability used in the WDW-163 lateral model.

In this model, the weighted average vertical permeability, k_z, of the containment interval is again calculated using the method of Domenico and Schwartz (1990),

$$k_z = \Sigma\, b_i / \Sigma\, (b_i / k_i) \qquad \text{(Eq. 7.2)}$$

The weighted average permeability, k_z, is:

$$kz = \frac{975\,ft + 1{,}110\,ft}{\dfrac{975\,ft}{4.4 \times 10^{-4} mD} + \dfrac{1{,}110\,ft}{1{,}600\,mD}} = 9.4 \times 10^{-4} mD$$

This value was converted to a hydraulic conductivity of 6.33×10^{-6} feet per day with the following equation:

$$K = \frac{(0.00094\text{ mD})(64.51\text{ lb/ft}^3)(86{,}400\text{ sec/day})(1\text{ darcy})(1.06\times10^{-11}\text{ ft}^2\text{/darcy})}{(0.42\text{ cP})(2.088\times10^{-5}\text{ lb-sec/ft}^2\text{-cP})(1{,}000\text{ mD})}$$

$$K = 6.33 \times 10^{-6}\text{ feet/day}$$

The weighted average vertical hydraulic conductivity, Kz, is 6.33×10^{-6} feet/day using the formation fluid density of 64.51 lb/ft^3, and a formation fluid viscosity of 0.42 cP at 182 °F).

WDW-164 Injection Interval Vertical Hydraulic Conductivity

The containment interval for the WDW-164 Injection Interval vertical model is based on the same average permeability values from Anahuac and upper Frio sands and shales as described above. This containment interval is approximately 2,720 feet thick, and contains 385 feet of Anahuac shale, underlain by 2,335 feet of inter-bedded Frio sand and shale strata, which overlays the WDW-164 Injection Interval. The permeability values chosen for the containment interval sands and shales are the same as described above. The 2,335 feet thick containment interval consists of approximately 1,045 feet of shale, plus approximately 1,675 feet total thickness of sand. The shale strata are conservatively estimated shale have permeabilities averaging 4.4×10^{-4} mD (discussed above), while the sand strata are conservatively estimated to have a vertical permeability of 1,600 mD, equal to the maximum permeability used in the WDW-163 lateral model.

In this model, the weighted average vertical permeability, k_z, of the containment interval is calculated using the method of Domenico and Schwartz (1990),

$$k_z = \Sigma\, b_i / \Sigma\, (b_i / k_i) \qquad \text{(Eq. 7.2)}$$

The weighted average permeability, k_z, is:

$$kz = \frac{1{,}045\, ft + 1{,}675\, ft}{\dfrac{1{,}045\, ft}{4.4 \times 10^{-4} mD} + \dfrac{1{,}675\, ft}{1{,}600\, mD}} = 1.1 \times 10^{-3} mD$$

This value was converted to a hydraulic conductivity of 7.76×10^{-6} feet per day with the following equation:

$$K = \frac{(0.0011 \text{ mD})(64.34 \text{ lb/ft}^3)(86{,}400 \text{ sec/day})(1 \text{ darcy})(1.06\times10^{-11} \text{ ft}^2\text{/darcy})}{(0.40 \text{ cP})(2.088\times10^{-5} \text{ lb-sec/ft}^2\text{-cP})(1{,}000 \text{ mD})}$$

$$K = 7.76 \times 10^{-6} \text{ feet/day}$$

The weighted average vertical hydraulic conductivity, Kz, is 7.76×10^{-6} feet/day using the formation fluid density of 64.34 lb/ft^3, and a formation fluid viscosity of 0.40 cP at 192 °F).

7.3.3 Porosity

Porosity of the Lateral Models

Based on the core analyses gathered during the drilling of WDW-163, WDW-164, and WDW-165 (presented in Section 4.3.2 and detailed below), an average porosity value of 34 percent was utilized as a representative value for the porosity of the modeled WDW-163 Injection Interval, 30 percent was utilized as a representative value for the porosity of the modeled WDW-164 Injection Interval, and an average porosity value of 28 percent was utilized as a representative value for the porosity of the modeled WDW-165 Injection Interval. The lateral model porosity values of 34 percent, 30 percent, and 28 percent for the WDW-163, WDW-164, and WDW-165 Injection Intervals respectively are the same as those used for the initial 1990 Petition and 1994 Petition re-issuance approvals. These values were derived from whole and sidewall core analyses from the three Ineos injection wells, as previously discussed in Sections 4.3.2 and 7.3.2.1.

The WDW-163 Injection Interval porosity range from whole core data is 30.3-41.9 percent (15 cores from WDW-163; see Appendix E cores from 5,375-5,614 feet), and from sidewall core data is 23.2-32.9 percent (7 cores from WDW-163 and 4 cores from WDW-165; see Appendix E cores from 5,425-5,700 feet and 5,410-5,680 feet respectively). The whole core porosity average is 40.0 percent, and the sidewall core average is 28.0 percent. The average of these two values is 34 percent, which is the value used in the lateral SWIFT modeling for the WDW-163 Injection Interval. This average porosity value also matches the average porosity as seen from the open hole neutron-density log from WDW-163 (included in Appendix D), which indicates a range of 30-38 percent and an average of 34 percent over the WDW-163 Injection Interval.

The WDW-164 Injection Interval porosity range from whole core data is 26.9-37.9 percent (16 cores from WDW-164; see Appendix I page 3 of 33, cores 2-17 and 28), and from sidewall core data is 20.1-32.3 percent (26 cores from WDW-164; see Appendix E cores from 7,436-7,970 ft). The whole core porosity average is 33.1 percent, and the sidewall core average is 27.7 percent. The average of these two values is 30 percent, which is the value used in the lateral SWIFT modeling for the WDW-164 Injection Interval.

The WDW-165 Injection Interval porosity range from whole core data is 29.7-36.4 percent (12 cores from WDW-164; see Appendix I page 3 of 33, cores 18-27 and 29-30), and from sidewall core data is 21.6-32.5 percent (16 cores from WDW-164 and 33 cores from WDW-165; see Appendix E cores from 6,806-7,404 feet and 6,800-7,435 feet respectively). The whole core porosity average is 32.9 percent, and the sidewall core average is 27.3 percent. The average of these two values is 30 percent, which is slightly above the 28 percent value used in the lateral SWIFT modeling for the WDW-163 Injection Interval. However, the lateral modeling porosity value used (28 percent) is conservative, as it results in less available sand pore space and a resultant plume which moves further over the modeling timeframe. In the pressure model, the lower porosity results in a higher pressure buildup at the well, which is also conservative.

Porosity of the Vertical Models

In the vertical models, a conservative porosity of 28 percent was assigned to the containment interval sand strata, and 10 percent to the shale strata. The sand porosity chosen is the lowest of the three used for the lateral model sands. The shale value is based on published values for Gulf Coast shales. Freeze and Cherry (1979) state that porosity values representative of shales range from 0 to 10 percent. Magara (1969), Price (1976), and Overton and Timco (1969) indicate that shales in the Gulf Coast region have an interconnected porosity of 10 to 20 percent. The 10 percent value was used in the previous Petition re-issuance modeling for the Green Lake facility (Intera, 1994), and will continue to be used for the vertical models.

In the vertical models, the weighted average porosity, ϕz, of the containment interval is calculated using the method of Domenico and Schwartz (1990),

$$\phi z = \Sigma\ bi / \Sigma\ (bi / \phi i) \qquad \text{(Eq. 7.3)}$$

$$\varphi z = \frac{445\,ft + 252\,ft}{\dfrac{445\,ft}{0.10} + \dfrac{252\,ft}{0.28}} = 13.0\,\%$$

The weighted average porosity is assumed homogeneous (no variation in porosity along the vertical path). Additionally, since the vertical model is one-dimensional (vertically upward), the weighted average porosity is assumed to be isotropic.

7.3.4 Lateral and Transverse Dispersivity

The longitudinal and transverse dispersivities used in the Ineos models are given in Tables 7-2a, 7-2b, and 7-2c. For the lateral models, the base case longitudinal dispersivity value of 160 feet was chosen from a compilation of data from many field sites throughout the world provided by Gelhar and others (1992) (included in Appendix K). The scale dependency of dispersivity is generally thought to be caused by macroscopic aquifer heterogeneity (Davis and others, 1985; and Adams and Gelhar, 1992). However, studies suggest that near the source, dispersivities increase with distance from the source until an asymptotic value is reached at the Taylor or Fickian limit. This is the limit at which dispersion becomes essentially a Fickian process and can be adequately described by the advection dispersion equation (Gelhar and others, 1979). In the field, the Taylor limit is considered to be reached on the order of 10s or 100s of feet from the source and after a time period of 10s to 100s of days (Anderson, 1984).

There is no clear consensus on how the dispersivity changes with plume scale. Therefore, it is appropriate and conservative to use an approach that falls in the middle of published results. This can be achieved by using the graph of equation 12b as depicted in Figure 1 of Xu and Eckstein (1995) (Appendix K). The fit of equation 12b falls significantly below Neuman's regression line. Therefore, justification exists for the use of much larger dispersivity values. The scales of the three Injection Interval model plumes for Ineos are on the order of 6,000 to 8,000 meters. This means that the use of a more conservative 160 feet for the longitudinal dispersivity in the Ineos models is justified, because from Figure 1 of Xu and Eckstein (1995) a larger value could be used. The base longitudinal dispersivity value of 160 feet is appropriate given the range of values reported for the spatial and temporal scales of the lateral models.

Regarding the transverse horizontal dispersivity, the Ineos models use a value of 16 feet which is one tenth of the longitudinal dispersivity. Gelhar and others (1992; p. 1970) (Appendix K) state that although a ratio of longitudinal to transverse dispersivity of 3 to 1 is commonly used in models, there is no support for this assumption. Figure 6 of Gelhar and others (1992) is included in Appendix K. Gelhar and others (1992) state that the data support a longitudinal to transverse dispersivity ratio of one order of magnitude or greater. This is also reasonable and conservative given the accepted ratio of transverse to longitudinal dispersivity of 0.01 to 0.5 (MacKay and others, 1985; Anderson, 1984). Therefore, the 10 to 1 ratio of longitudinal to transverse dispersivity ratio used in the Ineos models is valid and conservative.

Dispersivity was not considered in the vertical model for two reasons. First, the vertical transport is modeled conservatively as one-dimensional; no transverse component of advection or diffusion was allowed (these would dilute the waste as it moves upward). The result is that the waste movement is maximized. Second, at the end of the operational period when the Injection Interval pressurization has subsided, it is assumed that there is no additional potential for fluid flow in any direction; diffusion is the only transport mechanism. The result is a zero fluid velocity and therefore, no dispersion, since dispersion is the product of the fluid velocity and dispersivity.

7.3.5 Molecular Diffusivity

Molecular diffusion is modeled by considering the movement of a conservative electrolyte species in a porous medium. In SWIFT, the relationship between the effective and free solution (in water) molecular diffusivity is:

$$D = D_0 n \tau$$

where D is the effective molecular diffusivity in a porous medium, D_0 is the molecular diffusivity in water, n is the porosity, and τ is the tortuosity.

Molecular diffusion is included in both the lateral and vertical models to account for transport facilitated by the concentration gradient of the injectate. The molecular diffusivity for acrylamide was chosen for utilization in the lateral models because acrylamide is the constituent with the greatest concentration reduction factor (4.0×10^9) required to reach health based limits of all of the petitioned hazardous constituents which comprise the Ineos injected waste stream, as shown in Table 6-1. Acrylamide has a free water molecular diffusivity of 8.56×10^{-6} cm^2/sec. The bulk (free liquid) diffusion coefficient for acrylamide was determined using the Wilke-Chang equation (Johnson and others, 1989; see Appendix K):

$$\frac{D1_0}{D2_0} = \left[\frac{MW_2\rho_1}{MW_1\rho_2}\right]^{0.6} \qquad \text{(Eq. 7.4)}$$

where Dl_0 and $D2_0$ are the free solution (in water) molecular diffusivity of the compound of interest and the molecular diffusivity in water of a reference compound (benzene in this case), respectively. MW_1 and MW_2 are their molecular weights and ρ_1 and ρ_2 are the densities of the compounds at their boiling points. The densities and molecular weights were obtained from DHHS (1990; see Appendix K). The use of densities at standard temperatures results in molecular diffusivities that are within 10 percent of experimental values (Johnson and others, 1989). The molecular diffusivity in water for acrylamide (the component of the Ineos waste stream that has the highest concentration reduction factor) is:

$$D_0\,(\text{acrylamide}) = 7\,x\,10^{-10}\,\frac{m^2}{\sec}\left[\frac{\left(78.1\,\dfrac{g}{mole}\right)\left(1.12\,\dfrac{g}{cm^3}\right)}{\left(71.08\,\dfrac{g}{mole}\right)\left(0.88\,\dfrac{g}{cm^3}\right)}\right]^{0.6}$$

$$D_0\,(\text{acrylamide}) = 8.56 \text{ x } 10^{-10}\,\frac{\text{m}^2}{\sec}$$

The free-water diffusivity for acrylamide is $8.56 \text{ x } 10^{-6}$ cm^2/sec. This is equivalent to $7.96 \text{ x } 10^{-4}$ ft^2/day.

The effective molecular diffusion coefficient, D^* (required by SWIFT in the lateral models) for the Injection Interval is found by multiplying the bulk coefficient by the Injection Interval porosity and the tortuosity. The Injection Interval porosities are 34 percent, 30 percent, and 28 percent, respectively for the three Injection Intervals, as determined from Ineos core data. The tortuosity coefficients were assumed to be equal to the sand porosities of each Injection Interval (based on Miller, 1989, see Appendix K; Lerman 1988):

$$\begin{aligned} D^* &= 7.96 \text{ x } 10^{-4} \text{ ft}^2\text{/day x } 0.34 \text{ x } 0.34 \text{ (WDW-163)} \\ &= 9.20 \text{ x } 10^{-5} \text{ ft}^2\text{/day (WDW-163)} \end{aligned}$$

$$D^* = 7.96 \times 10^{-4}\ ft^2/day \times 0.30 \times 0.30\ (WDW\text{-}164)$$
$$= 7.16 \times 10^{-5}\ ft^2/day\ (WDW\text{-}164)$$

$$D^* = 7.96 \times 10^{-4}\ ft^2/day \times 0.28 \times 0.28\ (WDW\text{-}165)$$
$$= 6.24 \times 10^{-5}\ ft^2/day\ (WDW\text{-}165)$$

In the vertical transport model, the effective diffusion coefficient for transport of acrylamide through the overlying containment interval is determined using a tortuosity of 0.1, equal to the containment interval shale porosity:

$$D^* = 7.96 \times 10^{-4}\ ft^2/day \times 0.1$$
$$= 7.96 \times 10^{-5}\ ft^2/day$$

In the vertical transport model, the calculated free water diffusion coefficients are used for transport of acrylamide and the other constituents through the overlying containment interval. In the vertical transport model, the worst-case constituent movement is associated with selenium, which does not have the greatest concentration reduction factor, but has the worst-case diffusion coefficient. This results in the worst-case vertical diffusive movement (see Section 7.5.2).

The molecular diffusion of acrylamide and the other constituents through a mud-filled borehole was determined using their free water diffusivities as calculated above, and a tortuosity value of 0.5. This tortuosity value is chosen to reflect the tortuosity of the mud column, where the clay particles provide a substantial tortuosity effect.

Miller (1989; included in Appendix K) notes that plate-like clay particles provide a geometrical correction factor (tortuosity) on the order of four or more times greater than spherical particles. Slurries of montmorillonite clay minerals have been shown (Figure 7 of Miller, 1989) to have tortuosity values from 0.08 to 0.9, depending on the porosity of the mixture. Drilling muds (primarily composed of montmorillonite clays) have solid percentages by volume ranging from 3 to 30 percent (Magcobar, 1980; see Appendix K), which would result in porosity values for the mud column of 70 to 97 percent. If one applies these porosities to Figure 7 of Miller (1989), the resulting geometric correction factor (tortuosity) varies from 0.2 to 0.9. However, on average, the typical bentonite (sodium montmorillonite) mud (as typically used in the Gulf Coast) contains 10 percent solids by volume (Magcobar, 1980), with an equivalent 90 percent porosity. The choice of a tortuosity of 0.5 for a mud column is based on this use of a mud column porosity of 90 percent, which on Figure 7 would result in a tortuosity equal to 0.5. Pearce (1989; included in Appendix K) notes, in a review of the re-entry of a Gulf Coast mud-plugged well some 29 years later, that although the mud column density did not appreciably change in that time period, the gel strength did significantly increase. This is significant in that the increasing gel strength reflects the alignment of clay particles into an interconnected plated arrangement, greatly increasing the tortuous pathway for vertical movement of modeled contaminant particles (Figure 4 of Miller, 1989). Thus a smaller (<0.5) tortuosity value could be justified, and the 0.5 value used in the modeling is conservative.

Molecular diffusion is modeled conservatively given that the ion exchange capability of the clay minerals present in the shales and the sorption capacity of the residual carbon in the shale are ignored. Ion exchange and sorption are processes that will act to retard movement. As effective molecular diffusivity, which includes the effects of the porous media, is proportional to porosity and tortuosity increases with decreasing porosity, the molecular diffusivity in deep shales is often half that of shales buried at shallower depths. Therefore, the assignment of a porosity value of 10 percent for shales in the SWIFT models provides a valid input for the 10,000-year vertical simulation calculation.

The molecular diffusivity chosen and the modeling method employed are also conservative because Ineos has not considered chemical fate or hydrolysis in the modeling. These processes are expected to have a significant influence in reducing waste plume concentrations in a 10,000-year timeframe.

The molecular diffusivity used in the lateral modeling is for the worst-case constituent acrylamide, which has the greatest concentration reduction factor. Although other constituents listed in Table 7-6 may have larger calculated molecular diffusivities as shown on that table, their concentration reduction factors are generally an order of magnitude or more lower than that for the modeled constituent acrylamide.

Molecular Diffusion Through Shale

The molecular diffusion of acrylamide through shale was determined using the Do of 8.56 x 10^{-6} cm^2/sec calculated above, and a tortuosity of 0.10. The other constituents also use their calculated Do values and a tortuosity of 0.10. The tortuosity value is assumed to be approximately equal to the shale porosity.

Molecular Diffusion Through a Mud Filled Borehole

The molecular diffusion of acrylamide through a mud filled borehole was determined using the Do of 8.56 x 10^{-6} cm^2/sec calculated above, and a tortuosity of 0.5. The other constituents also use their calculated Do values and a tortuosity of 0.5. This tortuosity value is chosen to reflect the tortuosity of the mud column, where the clay particles provide a substantial tortuosity effect.

7.3.6 Modeled Injection Rates

There is only one Ineos injection well used in each of the three lateral models, as all three wells are within 1,000 feet of each other and each modeled well has its own Injection Interval. The injection history begins in 1981 with initiation of injection into WDW-165, followed by injection in 1982 in WDW-164, and injection in 1984 into WDW-163. The injection histories in the models continue through the end of 2007 for all three wells. A tabulation of the historical injection volumes is included as Table 7-4. For the future injection rates, the maximum permitted injection rates of 500 gpm each for the WDW-163, WDW-164, and WDW-165 Injection Intervals are used in the projected operational period from 1/1/2008 to 12/31/2017.

Documentation of these values is included in Appendix L in the form of State of Texas reports for the wells. The injection rates used in the models are also listed in Appendix L as injection rate summary tables. A discussion of each well's completion history is provided in Section 5.0. Future injection into each Injection Interval model is at a rate of 500 gpm for that respective well (WDW-163, WDW-164, or WDW-165) for a projected period of 10 years (2008 through 2017).

7.3.7 *Modeled Brine and Injectate Fluid Densities*

Formation Brine Densities

The formation fluid densities for the three Frio Injection Intervals was calculated based on a comparison of a measured Frio native brine sample obtained during the drilling of the WDW-163 well in 1983 from a depth of approximately 5,650 feet (within Sand 4 of WDW-163 Injection Interval), and on a previous Petition-referenced density value. That Petition-referenced December 1983 brine sample indicated that the Frio Formation native brine has an estimated total dissolved solids (TDS) content of approximately 86,700 mg/L at surface temperatures and pressures (Intera, 1994; see Appendix I). Appendix I also includes a WDW-163 formation brine analysis (page 4 of 14 of a 1994 Core Laboratories compatibility study report), which is summarized in Table 4-2, plus the Intera (1994; page 5-28) reference. Although the constituents listed in Table 4-2 (from the Core report) total to a TDS value of 81,912 mg/L, the higher value as quoted in the Intera (1994) document as being from a December 1983 collected brine sample is used in the modeling to maximize light plume movement over 10,000 years. There is some uncertainty as to whether the Core Laboratories report brine composition tabulation on page 4 of 14 of that document included all dissolved ions, or just those used to make up their synthetic brine also listed on that page (with a TDS value of 84,956 mg/L). Due to a lack of an original laboratory analytical results sheet for either referenced analysis, the higher Intera-referenced TDS value (included in Appendix I) extracted from the 1994 Petition document is used in the current Petition modeling. The other two Injection Intervals are assumed to have similar TDS values, as no native brine samples were gathered during the drilling of these wells, and the depositional environments are considered similar.